Energy Systems Department
Physical and Engineering Sciences Center

Diversifying Our Energy Supply

National energy security requires a robust portfolio of energy sources and the technologies to use them efficiently. In Sandia's Energy Systems Department, we are developing advanced alternatives to petroleum fuels and traditional energy supplies. For the transportation sector, we play leading roles in Department of Energy (DOE) programs to develop biofuels from lignocellulosic feedstocks and hydrogen storage materials for fuel cell vehicles. For the power production and end-use sectors, we are engineering new nanoporous materials that promise performance breakthroughs for batteries, supercapacitors, and other energy storage and conversion technologies.

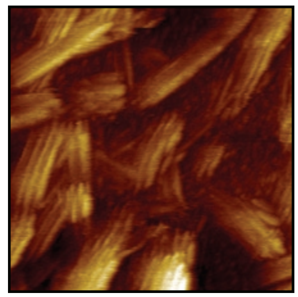
Our group encompasses multidisciplinary skills and backgrounds—in chemistry, biochemistry, materials science, computational science, physics, and chemical engineering—enabling a cross-cutting approach that rapidly assesses possibilities to focus on the most promising ideas. We partner with other Sandia departments as well as other national laboratories, industry, and academia to quickly realize practical solutions to national energy problems and goals.

Biofuel Conversion

We are developing cost-effective processes for converting biomass—both lignocellulosic and algal—into combustible fuel for transportation.

Lignocellulosic biomass, such as grasses and agricultural residue, is readily available on a sustainable basis. Unlike the starch from corn, however, it is a complex material that is significantly harder to convert into ethanol. This complexity requires innovative solutions for "deconstructing" the initial feedstock into fermentable sugars.

Efficient deconstruction calls for a detailed understanding of the interdependent roles played by biomass structure and chemical composition. We are using atomic force microscopy, confocal microscopy, and electron microscopy to study how biomass structure degrades under different pretreatment and enzymatic process environments. At the same time, we're evaluating cellulosic chemistry using Raman, FTIR, and fluorescence spectroscopy to better understand the relevant chemical linkages that give rise to recalcitrant biomass.



Atomic force microscopy image of recrystallized cellulose (taken in situ)

In addition to conducting our internal research on biomass deconstruction, we are part of DOE's new Joint BioEnergy Institute (JBEI, www.jbei.org), where we're leading research on the molecular mechanisms controlling the breakdown of lignocellulose into fermentable sugars and aromatics.

Algae are another potentially rich source of biofuel. Our group is developing more efficient methods of extracting oils from algae and converting them into high-purity transportation fuels. We use our skills in chemistry, chemical engineering, and mechanical engineering to transfer ideas to reality in proof-of-concept experiments, actively collaborating with industry to transition these advances to the transportation fuel sector.

Metal Hydrides for Hydrogen Storage

A key technical hurdle for fuel cell vehicles is the ability to carry sufficient hydrogen onboard to meet DOE FreedomCar criteria. Solid metal hydrides show great promise for this function, as they can reversibly absorb hydrogen into the interstitial spaces of their crystal lattices and release the hydrogen when needed.

To pursue this concept, DOE established the Metal Hydride Center of Excellence (MHCoE), which leverages the talent of six national laboratories, nine universities, and four private companies, organized into collaborative research teams that explore different approaches to creating a viable metal hydride storage material.

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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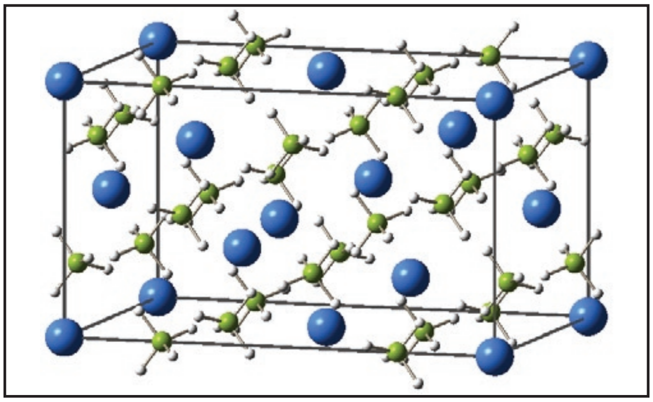
Our department manages the overall MHCoE on behalf of DOE. In addition, we're leading MHCoE research on complex anionic materials—i.e., complex anions embedded in a stabilizing matrix of cations.

One promising anionic material is catalyzed calcium borohydride, which we have prepared via a new synthesis route. We continue to search for high-capacity materials with a focus on ternary metal hydrides, which feature higher hydrogen content than intermetallic compound hydrides.

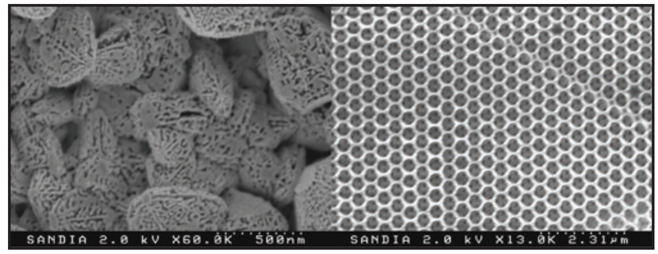


Crystal structure of $Ca(BH_4)_2$ as determined by synchrotron X-ray diffraction. This metal hydride was designed, synthesized, and characterized by our group.

To accelerate the discovery of superior hydrides, we rely on sophisticated simulation techniques such as a Monte Carlo structure-searching algorithm that minimizes electrostatic energy to screen for new compounds based on MH_X anions and a collection of corresponding cations. We then investigate the top candidates more thoroughly with density functional theory calculations and synthesize the most promising among them.

Nanoporous Materials for Energy Storage

It takes a few minutes to refuel an SUV, but closer to an hour to recharge an iPod or cell phone. A main reason is that high-capacity storage devices such as batteries rely on ions to carry electrical charge, which can be a very slow process, especially when the ions must travel through the long, narrow channels that provide high surface area in these devices.



Left: SEM image of a porous gold film. Right: SEM image of a periodic silica template for porous materials.

Our group is conducting fundamental science into numerous aspects of nanopore behavior, with a view to developing systematic modeling and synthesis methods that will allow us to rationally tune the architecture of nanomaterials—and thereby permit major performance advances in charging rate.

Moreover, optimally designed nano-architecture will enable dramatic improvement in electrical storage capacity, with ramifications for numerous advanced technologies.

For example, large jolts of energy often must be converted from one form to another and back again, as when a car stops at a light or a train stops at a station and then accelerates. Or, affecting the power grid, a gust of wind gives a burst of power to a turbine or a cloud passes over a solar cell, and moments later someone calls an elevator or starts a washing machine. Currently, there are major limitations on our ability to capture a surge of electrical energy, store it, and feed it back when needed. Nanopore design of materials could offer breakthrough levels of performance improvement in these technologies.

Control over pore structure is also likely to enhance other energy-related applications—for example, by allowing fuel cell membranes with mechanical and transport properties that vary less with changes in temperature, and fuel cell electrodes that make maximum use of catalyst particles due to optimal transport of reactants to the catalyst.

In addition to our fundamental studies of nanoporosity, we are currently developing nanomaterials relevant to hydrogen storage, supercapacitors, and electro-catalysis applications.

Learn more at: http://public.ca.sandia.gov/8700

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